2-Methoxyethyl acetate

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1	1	0-49-6	D.	TX	SI	D2	02	55	5

Model Performance

Model	Data

Weighted KNN model

5-fold CV (7	5%)	Training (75	5%)	Test (25%)	Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE		
0.85	1.14	0.85	1.12	0.83	1.23		

Model Results

Predicted value: 4.77e-12 cm3/molecule*sec

Global applicability domain: Inside

Local applicability domain index: 6.53e-01

Confidence level: 8.26e-01

Nearest Neighbors from the Training Set

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2-Ethoxyethyl acetate Measured: 1.30e-11 Predicted: 1.03e-11

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Ethyl lactate
Measured: 3.90e-12
Predicted: 4.80e-12

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Methyl 2-hydroxypropanoate **Measured:** 2.80e-12

Predicted: 3.16e-12

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Propyl acetate
Measured: 3.40e-12
Predicted: 2.52e-12

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Isopropyl acetate Measured: 3.40e-12 Predicted: 2.54e-12